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AN EFFICIENT HYBRID ANALYTICAL APPROACH, TO FILM PORE DIFFUSION MODEL USING WAVELETS

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ABSTRACT

In this paper, we have applied a new Chebyshev wavelet based coupled method to film-pore diffusion model. We have used the film-pore diffusion model, satisfactorily describe kinetics of methylene blue adsorption onto the three low-cost adsorbents, Gauva, teak and gulmohar plant leaf powders. We first discretize the nonlinear PDE and then utilized the Chebyshev wavelets on the obtained discretize nonlinear differential, equation to get the solution at each approximation of Picard method. The proposed wavelet based results are compared with the results, obtained by method of lines (MOL) and experimental results. Satisfactory agreement with the experimental and MOL results is observed.

KEYWORDS: Methylene blue, Adsorption Kinetics, Film-Pore Diffusion Model, Low-Cost Adsorbents, Chebyshev Wavelets & Picard Method

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Original Article

1. INTRODUCTION

Large amounts of dyes are utilized by textile industry and a significant portion of these dyes are not consumed in the process and therefore let out with the effluent. In recent years, the cost of commercial adsorbents is too high; interest for using low-cost adsorbents for removal of dyes from textile effluents is continuously growing. A recent survey indicates that, in India, on an average fresh water consumed and effluent generated per kg of finished textile are 175 L and 125 L, respectively [1] [Ponnusami et al 2010]. The presence of dyes in aqueous effluents is highly objectionable, as this affects the photosynthetic activity in receiving water body by reducing/preventing light penetration. As the dyes are recalcitrant in nature it is difficult to treat them, in conventional biological treatment plant [2, 3] [Ponnusami et al. 2007, Ponnusami et al. 2009]. Various researchers have worked on biological degradation of dyes. But, very often, the metabolic intermediates are found to be more toxic than the original compound [4]. Therefore, identification of low-cost adsorbents is given more attention by the researchers recently, as commercial adsorbents like activated carbon are too costly. Few recent studies investigating application of low cost adsorbents are: jackfruit peel [5], pine apple stem [6], phoenix tree leaves [7], pomelo peel [8], shells of bittim [9], orange peel [10], broad been peels [11] etc.

In our previous research works, we investigated the feasibility and adsorption of MB onto three plant leaf powders namely guava leaf powder (GLP), teak leaf powder (TLP) and gulmohar leaf powder (GUL) [1]. Hariharan et al. [46], used the film-pore diffusion model (FPDM) to describe the kinetics of methylene blue adsorption onto GLP, TLP and GUL. Diffusion based kinetic models are too complex and they require rigorous solution methods. For many of the diffusion and kinetics models do not have analytical solutions. In our previous

work we had used method of lines to solve film-pore diffusion model and had shown that Film-pore model could describe the kinetics of adsorption of MB onto GLP, TLP and GUL [1]. Hariharan et al. [46], had applied the Haar wavelet method for the solution of the above model. In this work, we have proposed a wavelet based coupled method to film-pore diffusion model.

Recently, wavelet based methods become important tools, because of the properties of localization. Chebyshev wavelet method (CWM) is one of the earliest and simplest examples of what is known now as a compact, dyadic, orthonormal wavelet transform [12-24,26]. Recently, Hariharan and his co-workers [19-32] have applied the wavelet transform methods for solving differential equations arising in Engineering. Wavelet-Galerkin method (WGM) was successfully applied for solving the nonlinear differential equations [33, 34].

The basic idea of Chebyshev wavelet method is to convert the PDEs to a system of algebraic equations by the operational matrices of integral or derivative [35-45]. The main goal is to show how wavelets and multi-resolution analysis can be applied for improving the method in terms of easy implementability and achieving the rapidity of its convergence. In this work, we have applied a wavelet based coupled method, which combines the Picard's method and the Chebyshev wavelet method for the numerical solution of the film pore diffusion mode. To the best of our knowledge until now there is no rigorous Chebyshev-Picard wavelet solution has been reported for the above model.

2. MATERIALS AND METHODS

Film-pore diffusion model (FPDM) is successfully described earlier by McKay and co-workers [47, 48]. Numerical results of FPDM by method of lines are described in our previous paper [1]. Haar wavelet based solution of FPDM is described in our previous paper [46]. In the present paper, we have developed the Chebyshev-Picard wavelet method is described in detailed and the results are compared with our previous solution.

2.1. Wavelet Preliminaries

Wavelets are the family of functions which are derived from the family of scaling function { $\emptyset_{j,k:}\ k \in Z\}$ where:

$$\emptyset(x) = \sum_k a_k\ \emptyset(2x - k) \tag{2.1}$$

For the continuous wavelets, the following equation can be represented:

$$\Psi_{a,b}(x) = |a|^{\frac{-1}{2}}\Psi\left(\frac{x-b}{a}\right)\quad a, b \in R, a \neq 0. \tag{2.2}$$

Where a and b are dilation and translation parameters, respectively, such that $\Psi(x)$ is a single wavelet function.

The discrete values are put for a and b in the initial form of the continuous wavelets, i.e.:

$$a = a_0^{-j},\ a_0 > 1,\ b_0 > 1, \tag{2.3}$$

$$b = kb_0a_0^{-j},\quad j, k \in Z. \tag{2.4}$$

Then, a family of discrete wavelets can be constructed as follows:

$$\Psi_{j,k} = |a_0|^{\frac{j}{2}} \Psi(2^j x - k), \tag{2.5}$$

So, $\Psi_{j,k}(x)$ constitutes an orthonormal basis in L^2 (R), where $\Psi(x)$ is a single function.

2.2. Function Approximations and Chebyshev Wavelets

We can express any function $f(x) \in L^2[0,1)$ into truncated second kind Chebyshev wavelets series as indicated below.

A function $$f(x) = \sum_{n=1}^{2^{k-1}} \sum_{m=0}^{M-1} c_{nm} \psi_{n,m}(x) = C^T \Psi(x), \tag{2.6}$$

where C and $\Psi(x)$ are $2^{k-1}M \times 1$ matrices, given by the following column matrices.

$$C = \left[c_{10}, c_{11}, \ldots, c_{1,M-1}, c_{20}, c_{21}, \ldots, c_{2,M-1}, \ldots, c_{2^k,M-1} \right]^T,$$

$$\psi(x) = \left[\psi_{10}(x), \psi_{11}(x), \ldots, \psi_{1,M-1}(x), \psi_{20}(x), \ldots, \psi_{2,M-1}(x), \ldots, \psi_{2^k,0}(t), \ldots, \psi_{2^k,M-1}(x) \right]^T$$

Using the collocation points as following:

$$x_i = \frac{(2i-1)}{2^k M}, \quad i = 1, 2, \ldots, 2^{k-1} M.$$

We can define the Chebyshev wavelet matrix $\Psi_{m \times m}$ as:

$$\Psi_{m \times m} \square \left[\Psi\left(\frac{1}{2^k M} \right), \ \Psi\left(\frac{3}{2^k M} \right), \ldots \ \Psi\left(\frac{2^k M - 1}{2^k M} \right) \right].$$

For example, when $M = 3$ and $k = 2$ the Chebyshev wavelet is expressed as

$$\Psi_{6 \times 6} = \begin{bmatrix} 1.2732 & 1.2732 & 1.2732 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.2732 & 1.2732 & 1.2732 \\ -1.6977 & 0 & 1.6977 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1.6977 & 0 & 1.6977 \\ 0.9903 & -1.2732 & 0.9903 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.9903 & -1.2732 & 0.9903 \end{bmatrix}$$

2.3. Chebyshev Wavelets Operational Matrix of Integration

The integration of the vector $\Psi(t)$ defined in Eq. (8) can be obtained as

$$\int_0^t \Psi(s)ds \approx P\Psi(t), \tag{2.7}$$

where P is the $\left(2^k M\right)\times\left(2^k M\right)$ operational matrix for integration and is given as

$$P=\begin{pmatrix} C & S & S & \ldots & S \\ O & C & S & \ldots & S \\ O & O & C & \ldots & S \\ \vdots & \vdots & \vdots & \ddots & S \\ O & O & O & \cdots & C \end{pmatrix}$$

where S and C are $M \times M$ matrices given by:

$$S=\begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ -\frac{1}{3} & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ -\frac{1}{15} & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -\frac{1}{2M\left(M-2\right)} & 0 & 0 & \cdots & 0 \end{pmatrix}$$

and

$$C=\frac{1}{2^k}\begin{pmatrix} \frac{1}{2} & \frac{1}{2\sqrt{2}} & 0 & 0 & \cdots & 0 & 0 & 0 \\ -\frac{1}{8\sqrt{2}} & 0 & \frac{1}{8} & 0 & \cdots & 0 & 0 & 0 \\ -\frac{1}{6\sqrt{2}} & -\frac{1}{4} & 0 & \frac{1}{12} & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ -\frac{1}{2\sqrt{2}(M-1)(M-3)} & 0 & 0 & 0 & \cdots & -\frac{1}{4(M-3)} & 0 & -\frac{1}{4(M-1)} \\ -\frac{1}{2\sqrt{2}M(M-2)} & 0 & 0 & 0 & \cdots & 0 & -\frac{1}{4(M-2)} & 0 \end{pmatrix}$$

The integration of the product of two Chebyshev wavelet function vectors is obtained as

$$I=\int_0^1 \Psi(x)\Psi^T(x)\,dx, \tag{2.8}$$

where I is an identity matrix.

Theorem 2.1 (Accuracy estimation): Let $f(t)$ be a continuous function defined on $[0,1)$, with bounded second derivative $\left|f''(t)\right|$ bounded by B, and then we have the following accuracy estimation:

$$\sigma_{k,M} < \frac{\sqrt{\pi}B}{8}\left[\sum_{n=\mu^k+1}^{\infty}\frac{1}{n^5}\sum_{m=M}^{\infty}\frac{1}{(m-1)^4}\right]^{\frac{1}{2}}, \tag{2.9}$$

where

$$\sigma_{k,M} = \left[\int_0^1 \left(f(t) - \sum_{n=1}^{\mu^k} \sum_{m=0}^{M-1} c_{nm} \psi_{n,m}^{(k)}(t) \right)^2 w_n(t)\, dt \right]^{\frac{1}{2}}.$$

2.4. Convergence Analysis of the Proposed Method

In this section, we can derive an error bound of the Chebyshev wavelet Picard technique to an arbitrary unknown function.

Theorem 4.1: Let s, k and M tends to ∞, then the series solution Equation.(9) converges to $f(x)$.

Proof: Let $L^2[0,1)$ be the Hilbert space and $\psi_{n,m}$ forms a basis of $L^2[0,1)$. Consider

$$f_{s+1}(x) = \sum_{n=1}^{2^{k-1}} \sum_{m=0}^{M-1} c_{nm}^{s+1} \psi_{n,m}(x),$$

where

$$c_{nm}^{s+1} = \left\langle f_{s+1}(x), \psi_{n,m}(x) \right\rangle = \int_0^1 \sqrt{1-x^2}\, f(x) \psi_{n,m}(x)\, dx,$$

Let $R_{k,M}^{s+1}$ be a sequence of partial sums of $c_{nm}^{s+1}\psi_{n,m}(x)$, we prove that $R_{k,M}^{s+1}$ is a Cauchy sequence in Hilbert space $L^2[0,1)$ and then we show that $R_{k,M}^{s+1}$ converges to $f_{s+1}(x)$, when $k, M \to \infty$.

We show that $R_{k,M}^{s+1}$ is a Cauchy sequence. Consider $R_{\hat{k},\hat{M}}^{s+1}$ be arbitrary sums of $c_{nm}^{s+1}\psi_{n,m}^{s+1}$ with $k > \hat{k},\ M > \hat{M}$.

$$\begin{aligned}
\left\| R_{k,M}^{s+1} - R_{\hat{k},\hat{M}}^{s+1} \right\|^2 &= \left\| \sum_{n=1}^{2^{k-1}} \sum_{m=0}^{M-1} c_{nm}^{s+1} \psi_{n,m}(x) - \sum_{n=1}^{2^{\hat{k}-1}} \sum_{m=0}^{\hat{M}-1} c_{nm}^{s+1} \psi_{n,m}(x) \right\|^2 \\
&= \left\| \sum_{n=2^{\hat{k}-1}+1}^{2^{k-1}} \sum_{m=\hat{M}}^{M-1} c_{nm}^{s+1} \psi_{n,m}^{\mu}(x) \right\|^2 \\
&= \left\langle \sum_{n=2^{\hat{k}-1}+1}^{2^{k-1}} \sum_{m=\hat{M}}^{M-1} c_{nm}^{s+1} \psi_{n,m}(x),\ \sum_{i=2^{\hat{k}-1}+1}^{2^{k-1}} \sum_{j=\hat{M}}^{M-1} c_{ij}^{s+1} \psi_{i,j}(x) \right\rangle \\
&= \sum_{n=2^{\hat{k}-1}+1}^{2^{k-1}} \sum_{m=\hat{M}}^{M-1} \sum_{i=2^{\hat{k}-1}+1}^{2^{k-1}} \sum_{j=\hat{M}}^{M-1} c_{nm}^{s+1} c_{ij}^{s+1} \left\langle \psi_{n,m}(x), \psi_{i,j}(x) \right\rangle \\
&= \sum_{n=2^{\hat{k}-1}+1}^{2^{k-1}} \sum_{m=\hat{M}}^{M-1} \left| c_{nm}^{s+1} \right|^2
\end{aligned}$$

Using the Bessel's inequality, we have $\sum_{n=1}^{\infty}\sum_{m=0}^{\infty}\left|c_{nm}^{s+1}\right|^2$ is convergent and hence $\left\|R_{k,M}^{s+1}-R_{\widehat{k},\widehat{M}}^{s+1}\right\|^2 \to 0 \;\; as \;\; k,M,\widehat{k},\widehat{M} \to \infty$. This implies that $R_{k,M}^{s+1}$ is a Cauchy sequence and it converges to $y_{s+1}(x)\in L^2[0,1)$. It is enough to show that $y_{s+1}(x)=f_{s+1}(x)$.

$$
\begin{aligned}
\left\langle y_{s+1}(x)-f_{s+1}(x),\psi_{n,m}(x)\right\rangle &= \left\langle y_{s+1}(x),\psi_{n,m}(x)\right\rangle-\left\langle f_{s+1}(x),\psi_{n,m}(x)\right\rangle, \\
&= \underset{k,M\to\infty}{Lt}\left\langle R_{k,M}^{s+1},\psi_{n,m}(x)\right\rangle-c_{nm}^{s+1}, \\
&= c_{nm}^{s+1}-c_{nm}^{s+1}, \\
&= 0
\end{aligned}
$$

Hence $\sum_{n=1}^{2^{k-1}}\sum_{m=0}^{M-1}c_{nm}^{s+1}\psi_{n,m}(x)$ converges to $f_{s+1}(x)$ as $k,M\to\infty.$

Hence the theorem

3. METHOD OF SOLUTION BY THE CHEBYSHEV WAVELETS- PICARD METHOD (CWPM)

The film pore diffusion model is governed by a Reaction-diffusion-convection equation [1,46]

$$
\frac{\partial C}{\partial \tau}=A(C)\frac{\partial^2 C}{\partial z^2}+\frac{1}{z}\frac{\partial C}{\partial z} \tag{3.1}
$$

Where

$$
A(C)=\frac{1}{\varepsilon_p+\left(\frac{q_h\rho_p}{c_0}\right)\left(\frac{1+bc_0}{(1+bc_0C)^2}\right)}
$$

with initial conditions

$$
C(z,0)=e^{-z},C(z,1)=e^{-z-0.09},C(0,\tau)=e^{-0.09\tau},C(1,\tau)=e^{-1-0.09\tau} \tag{3.2}
$$

C-Concentration of the dye (methyline blue), τ-time variable, z-spatial variable, ε_p-particle porosity, ρ_p-particle density c_0 – initial bulk concentration

We apply the Picard technique to equation Equation.(3.1)

$$
\frac{\partial C_{s+1}}{\partial \tau}-A(C)\frac{\partial^2 C_{s+1}}{\partial z^2}=\frac{1}{z}\frac{\partial C_s}{\partial z} \tag{3.3}
$$

Where $s\in N, C_s(z,\tau)$ is known and this term can be used for obtaining $C_{s+1}(z,\tau)$

The initial and boundary conditions are

$$C_{s+1}(z,0)=e^{-z}, C_{s+1}(z,1)=e^{-z-0.09}, C_{s+1}(0,\tau)=e^{-0.09\tau}, C_{s+1}(1,\tau)=e^{-1-0.09\tau}$$

We can establish the Chebyshev wavelets method (CWM) to equation Equation.(3.3) as

$$\frac{\partial^2 C_{s+1}}{\partial z^2}=\sum_{L=1}^{\hat{m}}\sum_{i=1}^{\hat{m}} C_{L,j}^{r+1}\psi_L(z)\psi_i(z)=\psi^T(z)F^{s+1}\psi(\tau) \tag{3.4}$$

Apply the integral operator In_z^2 Equation.(3.4)

$$C_{s+1}(z,\tau)=In_z^2\psi^T(z)F^{s+1}\psi(\tau)+l_i(\tau)z+l_2(\tau) \tag{3.5}$$

Using the boundary conditions,

$$l_2(\tau)=0$$
$$l_1(\tau)=\frac{1}{b}\left[\left(I_{z=b}^{\beta}\psi^T(z)\right)F^{s+1}\psi(\tau)\right]$$

Equation.(3.5) becomes

$$C_{s+1}(z,\tau)=In_z^2\psi^T(z)F^{s+1}\psi(\tau)-x\left[In_{x=b}^{\beta}\psi^T(z)\right]F^{s+1}\psi(\tau) \tag{3.6}$$

Equation.(3.3) can be written as

$$\frac{\partial C_{s+1}}{\partial \tau}=A(C)\frac{\partial^2 C_{s+1}}{\partial z^2}+\frac{1}{z}\frac{\partial C_s}{\partial z} \tag{3.7}$$

With the help of Equation.(3.4), Equation.(3.7) becomes

$$\frac{\partial C_{s+1}}{\partial \tau}=A(c)\psi^T(z)F^{s+1}\psi(\tau)-\psi^T(z)N^{s+1}\psi(\tau) \tag{3.8}$$

where $N^{s+1}=\left(\psi^T(z)\right)^{-1}\left(\frac{1}{z}\frac{\partial C_s}{\partial z}\right)\left(\psi(\tau)\right)^{-1}$ (3.9)

Using the integral operator In_L^l to Equation.(3.9) and the initial conditions to obtain the following formula

$$C_{s+1}(z,\tau)=A(c)\psi^T(z)F^{s+1}\left(In_L^l\psi(\tau)\right)-\psi^T(z)N^{s+1}\left(In_L^l\psi(\tau)\right)+e^{-z}+e^{-z-0.09} \tag{3.10}$$

From Equation.(3.6) and Equation.(3.10), one can get

$$G\left[In_z^2\psi^T(z)-z\left[In_{z=b}^2\psi^T(z)\right]F^{s+1}-F^{s+1}\left[I_L^l\psi(\tau)(\psi(\tau))^{=1}+GF\,\psi(\tau)\right]^{-1}\right]=0 \tag{3.11}$$

Where, $G=\left(A(c)\psi^T(z)\right)^{-1}$ and $F=\left[-\left(-\psi^T(z)N^{s+1}\left(I_L^l\psi(\tau)\right)+e^{-z}+e^{-z-0.09}\right)\right]$

Equation.(3.11) is the Sylvester equation. We solve Eq.(3.11) for F^{s+1} and applying F^{s+1} in equations (3.6) or (3.10) to obtain the solution $C(z,\tau)$ at $(s+1)^{th}$ approximation of Picard iterative approach, at the collocation points.

Table.1: Comparison of CWPM, MOL and HWM by Obtaining the Mass Transfer Coefficients Using Film-Pore Diffusion Model Adsorption of MB onto GLP and k=1 and M=3. [$A(C_i)$ are Constants (linear) and $\in = 0.5$, $\rho = 500$]

Temp	C_0 $(mgdm^{-3})$	$k_f(ms^{-1})$ External- film transfer coefficient			$D_{eff}(m^2s^{-1})$ Internal effective diffusivity			Error		
K		MOL	HWM	CWPM	MOL	HWM	CWPM	E_M	E_H	E_C
303	50 100 150 200	$1.00\text{x}10^{-6}$	$3.00\text{x}10^{-6}$	$4.23\text{x}10^{-6}$	$1.74\text{x}10^{-13}$	$2.54\text{x}10^{-13}$	$1.24\text{x}10^{-13}$	1.197 0.140 0.935 1.61	0.938 0.129 0.824 1.102	0.638 0.029 0.483 0.873
313	50 100 150 200	$1.71\text{x}10^{-6}$	$3.45\text{x}10^{-6}$	$6.35\text{x}10^{-6}$	$6.46\text{x}10^{-13}$	$9.26\text{x}10^{-13}$	$7.32\text{x}10^{-13}$	1.462 1.120 1.267 7.570	1.221 0.927 1.016 5.112	1.112 0.653 0.820 3.234
323	50 100 150 200	$4.27\text{x}10^{-6}$	$4{,}75\text{x}10^{-6}$	$4.01\text{x}10^{-6}$	$3.11\text{x}10^{-13}$	$5.31\text{x}10^{-13}$	$4.54\text{x}10^{-13}$	0.856 0.160 2.168 3.164	0.28 0.000 1.208 1.016	0.192 0.000 0.727 0.523

4. CONCLUSIONS

In the present paper, we have successfully applied the CWPM for the film-pore diffusion model. It was investigated that the model could predict the concentration decay curve for all adsorption of methylene blue onto TLP, GUL and GLP excellently with a small deviation, during initial period. It gives better results when compared with the results by method of lines and Haar wavelet method. It is worth mentioning that, CWPM provides excellent results, even for small values of m. For larger values of m, we can obtain the results closer to the real values. The method with far less degrees of freedom and with smaller CPU time, provides better solutions than classical ones. The work confirmed the power of the CWPM, in handling nonlinear equations. This method can be easily extended to find the solution of all other non-linear diffusion equations too.

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